

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTACDR1614

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* \* \* \* \* Welcome to STN International \* \* \* \* \* \* \* \* \*

NEWS 1 Web Page for STN Seminar Schedule - N. America  
NEWS 2 APR 04 STN AnaVist, Version 1, to be discontinued  
NEWS 3 APR 15 WPIDS, WPINDEX, and WPIX enhanced with new predefined hit display formats  
NEWS 4 APR 28 EMBASE Controlled Term thesaurus enhanced  
NEWS 5 APR 28 IMSRESEARCH reloaded with enhancements  
NEWS 6 MAY 30 INPAFAMDB now available on STN for patent family searching  
NEWS 7 MAY 30 DGENE, PCTGEN, and USGENE enhanced with new homology sequence search option  
NEWS 8 JUN 06 EPFULL enhanced with 260,000 English abstracts  
NEWS 9 JUN 06 KOREAPAT updated with 41,000 documents  
NEWS 10 JUN 13 USPATFULL and USPAT2 updated with 11-character patent numbers for U.S. applications  
NEWS 11 JUN 19 CAS REGISTRY includes selected substances from web-based collections  
NEWS 12 JUN 25 CA/CAplus and USPAT databases updated with IPC reclassification data  
NEWS 13 JUN 30 AEROSPACE enhanced with more than 1 million U.S. patent records  
NEWS 14 JUN 30 EMBASE, EMBAL, and LEMBASE updated with additional options to display authors and affiliated organizations  
NEWS 15 JUN 30 STN on the Web enhanced with new STN AnaVist Assistant and BLAST plug-in  
NEWS 16 JUN 30 STN AnaVist enhanced with database content from EPFULL  
NEWS 17 JUL 28 CA/CAplus patent coverage enhanced  
NEWS 18 JUL 28 EPFULL enhanced with additional legal status information from the epoline Register  
NEWS 19 JUL 28 IFICDB, IFIPAT, and IFIUDB reloaded with enhancements  
NEWS 20 JUL 28 STN Viewer performance improved  
NEWS 21 AUG 01 INPADOCDB and INPAFAMDB coverage enhanced  
NEWS 22 AUG 13 CA/CAplus enhanced with printed Chemical Abstracts page images from 1967-1998  
NEWS 23 AUG 15 CAOLD to be discontinued on December 31, 2008  
NEWS 24 AUG 15 CAplus currency for Korean patents enhanced  
NEWS 25 AUG 25 CA/CAplus, CASREACT, and IFI and USPAT databases enhanced for more flexible patent number searching  
NEWS 26 AUG 27 CAS definition of basic patents expanded to ensure comprehensive access to substance and sequence information

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,  
AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

NEWS HOURS STN Operating Hours Plus Help Desk Availability

NEWS LOGIN      Welcome Banner and News Items  
NEWS IPC8      For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

FILE 'HOME' ENTERED AT 10:33:37 ON 08 SEP 2008

FILE 'REGISTRY' ENTERED AT 10:33:44 ON 08 SEP 2008  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 7 SEP 2008 HIGHEST RN 1047406-12-1  
DICTIONARY FILE UPDATES: 7 SEP 2008 HIGHEST RN 1047406-12-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

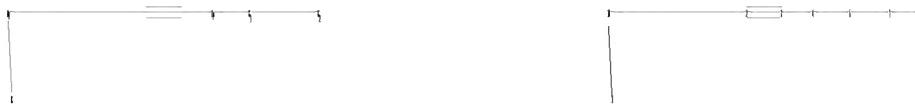
TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stnqen/stndoc/properties.html>

=>  
Uploading C:\Program Files\STNEXP\Queries\10596745s5.str



```

chain nodes :
1 2 3 4 6 7 9 10
chain bonds :
1-10 2-3 2-10 3-4 4-6 6-7 7-9
exact/norm bonds :
1-10 2-10 3-4 4-6 6-7 7-9
exact bonds :
2-3

```

G1:C,O,N

G2:C,O,N

```

Match level :
1:CLASS 2:CLASS 3:CLASS 4:Atom 6:CLASS 7:CLASS 9:CLASS 10:Atom
Element Count :
Node 10: Limited
    C,C4
    N,N2

```

L1           STRUCTURE UPLOADED

```

=> s l1 sss sam
SAMPLE SEARCH INITIATED 10:33:57 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 15428 TO ITERATE

```

```

13.0% PROCESSED       2000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

```

4 ANSWERS

```

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                          BATCH **COMPLETE**
PROJECTED ITERATIONS:     301120 TO 316000

```

PROJECTED ANSWERS:

284 TO

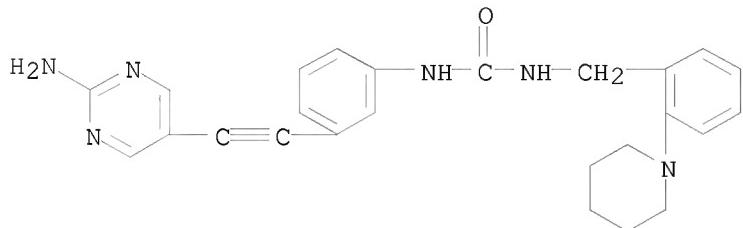
950

L2

4 SEA SSS SAM L1

=> d scan

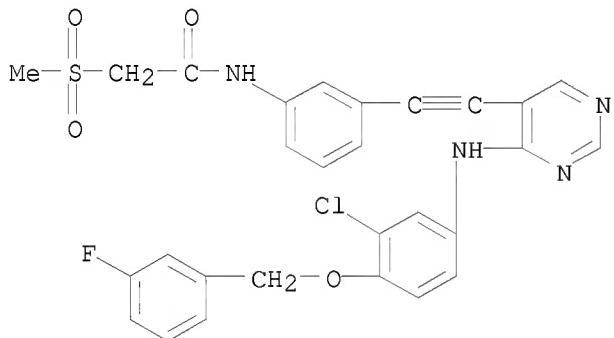
L2 4 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN  
IN Urea, N-[3-[2-(2-amino-5-pyrimidinyl)ethynyl]phenyl]-N'-[2-(1-piperidinyl)phenyl]methyl-  
MF C25 H26 N6 O



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

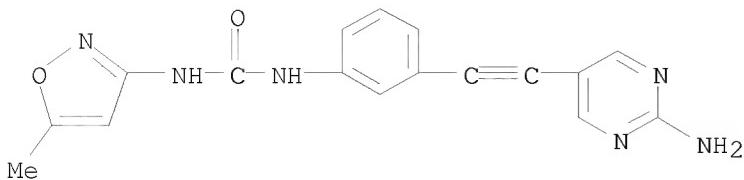
L2 4 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN  
IN Acetamide, N-[3-[2-[4-[(3-chloro-4-[(3-fluorophenyl)methoxy]phenyl]amino]-5-pyrimidinyl]ethynyl]phenyl]-2-(methylsulfonyl)-  
MF C28 H22 Cl F N4 O4 S



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

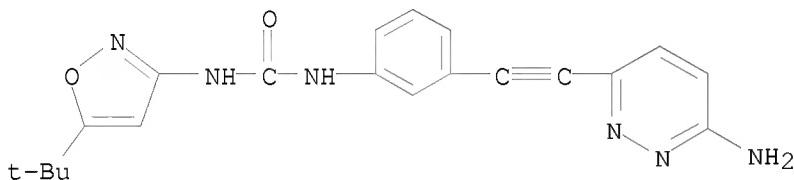
L2 4 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN  
IN Urea, N-[3-[2-(2-amino-5-pyrimidinyl)ethynyl]phenyl]-N'-(5-methyl-3-isoxazolyl)-  
MF C17 H14 N6 O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 4 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN  
 IN Urea, N-[3-[2-(6-amino-3-pyridazinyl)ethyl]phenyl]-N'-(5-(1,1-dimethylethyl)-3-isoxazolyl)-  
 MF C20 H20 N6 O2



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

ALL ANSWERS HAVE BEEN SCANNED

=> 1

1 IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system.  
 For a list of commands available to you in the current file, enter  
 "HELP COMMANDS" at an arrow prompt (>).

=> s ll sss full

FULL SEARCH INITIATED 10:35:00 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 308912 TO ITERATE

100.0% PROCESSED 308912 ITERATIONS  
 SEARCH TIME: 00.00.03

374 ANSWERS

L3 374 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

FULL ESTIMATED COST

ENTRY

SESSION

179.28

179.49

FILE 'CAPLUS' ENTERED AT 10:35:16 ON 08 SEP 2008

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 8 Sep 2008 VOL 149 ISS 11  
FILE LAST UPDATED: 7 Sep 2008 (20080907/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/legal/infopolicy.html>

=> s 13  
L4 18 L3

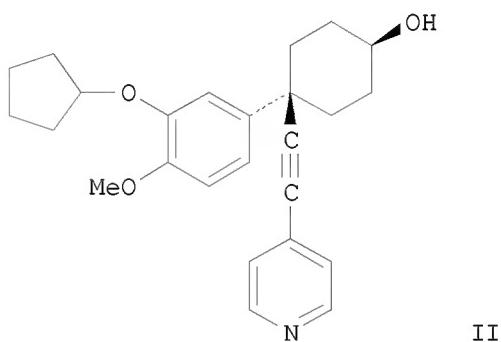
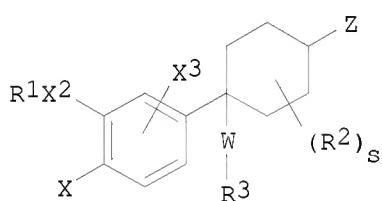
=> d ibib abs hitstr 18

L4 ANSWER 18 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 1996:531791 CAPLUS  
DOCUMENT NUMBER: 125:195045  
ORIGINAL REFERENCE NO.: 125:36527a,36530a  
TITLE: 4,4-(Disubstituted)cyclohexan-1-ol derivatives useful as PDE IV and TNF inhibitors  
INVENTOR(S): Christensen, Siegfried B., IV; Karpinski, Joseph M.; Ryan, M. Dominic; Bender, Paul E.  
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA  
SOURCE: PCT Int. Appl., 45 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9619988	A1	19960704	WO 1995-US16711	19951221
W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MN, MX, NO, NZ, PL, PT, RO, RU, SD, SG, SI, SK, TJ, TM, TT, UA, US, UZ, VN				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2208444	A1	19960704	CA 1995-2208444	19951221
AU 9646433	A	19960719	AU 1996-46433	19951221
AU 703246	B2	19990325		
ZA 9510878	A	19970617	ZA 1995-10878	19951221
EP 794774	A1	19970917	EP 1995-944363	19951221
EP 794774	B1	20051012		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
BR 9510257	A	19971104	BR 1995-10257	19951221
CN 1175210	A	19980304	CN 1995-197683	19951221
CN 1090020	C	20020904		

HU 77350	A2	19980330	HU 1997-2078	19951221
JP 10511658	T	19981110	JP 1995-520529	19951221
IL 116490	A	20010808	IL 1995-116490	19951221
AT 306260	T	20051015	AT 1995-944363	19951221
TW 412531	B	20001121	TW 1996-85103091	19960315
FI 9702676	A	19970819	FI 1997-2676	19970619
NO 9702906	A	19970815	NO 1997-2906	19970620
US 5891883	A	19990406	US 1997-860287	19970911
IN 1999DE01115	A	20050701	IN 1999-DE1115	19990817
PRIORITY APPLN. INFO.:			US 1994-363506	A 19941223
			US 1995-455866	A 19950531
			WO 1995-US16711	W 19951221
			IN 1995-DE2392	A3 19951222

OTHER SOURCE(S): MARPAT 125:195045  
GI



AB The invention relates to novel 4,4-disubstituted cyclohexan-1-ol derivs. I [R1 = various sidechains; X = YR2, F, (un)substituted NH2; Y = O, S(O)m; m = 0, 1, 2; X2 = O, (un)substituted NH; X3 = H, as given for X; R2 = (poly)(halo)methyl or -ethyl; s = 0-4; W = alk(en/yn)yl; R3 = CO2H or esters or amides, (hetero)aryl(alkyl), etc.; Z = OH, SH, NH2, and their derivs.; with provisos]. The compds. are useful for treating allergic and inflammatory diseases (especially asthma), for inhibiting the production of tumor

necrosis factor (TNF), as antivirals and antifungals, and for reducing toxicity of antimicrobials such as amphotericin B (no data). For example, 4-[3-(cyclopentyloxy)-4-methoxyphenyl]-4-ethynylcyclohexan-1-one was reduced by NaBH4, and the resulting cis- and trans-cyclohexanol derivs. were separated by flash chromatog. The trans-isomer was coupled with 4-bromopyridine using Pd(PPh3)4 and CuI to give title compound II. Prepns. of addnl. I and several related 3,3-disubstituted cyclohexanone derivs. are given.

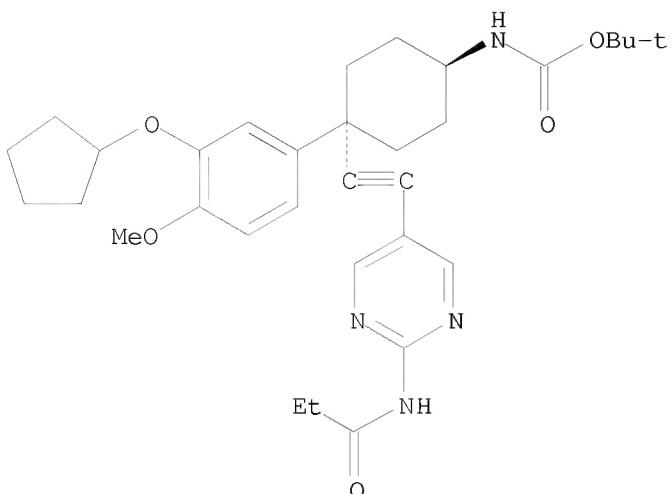
IT 180530-03-4P 180530-04-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(intermediate; preparation of cyclohexanol derivs. as PDE IV and TNF inhibitors)

RN 180530-03-4 CAPLUS

CN Carbamic acid, [4-[3-(cyclopentyloxy)-4-methoxyphenyl]-4-[[2-[(1-oxopropyl)amino]-5-pyrimidinyl]ethynyl]cyclohexyl]-, 1,1-dimethylethyl ester, trans- (9CI) (CA INDEX NAME)

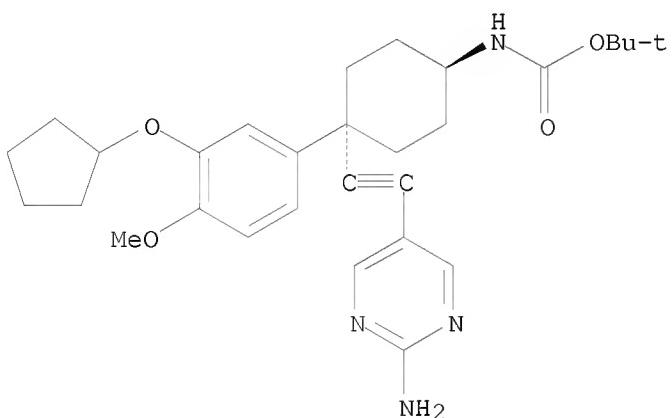
Relative stereochemistry.



RN 180530-04-5 CAPLUS

CN Carbamic acid, [4-[(2-amino-5-pyrimidinyl)ethynyl]-4-[3-(cyclopentyloxy)-4-methoxyphenyl]cyclohexyl]-, 1,1-dimethylethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



=> d ibib abs hitstr 17

L4 ANSWER 17 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:571772 CAPLUS

DOCUMENT NUMBER: 131:196102

TITLE: Nucleotide compounds including a rigid linker

INVENTOR(S): Khan, Shaheer H.; Rosenblum, Barnett B.; Zhen, Weiguo; Menchen, Steven M.

PATENT ASSIGNEE(S): USA

SOURCE: U.S., 32 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.

KIND DATE

APPLICATION NO.

DATE

US 5948648	A	19990907	US 1998-87250	19980529
US 6197555	B1	20010306	US 1999-461510	19991214
US 20020151711	A1	20021017	US 2002-85561	20020226
US 6653462	B2	20031125		
PRIORITY APPLN. INFO.:			US 1998-87250	A2 19980529
			US 1998-172789	A3 19981014
			US 1999-461506	A1 19991214

OTHER SOURCE(S): MARPAT 131:196102

AB A nucleoside/tide compound having a rigid linker attached to the 8-position of a purine, the 7-position of a 7-deazapurine and the 5-position of a pyrimidine is disclosed. Fluorescent dyes may be attached to this linker and the fluorescent nucleotide used in primer extension reactions. Thus, the fluorescein dye HEX-1 was attached to the 5-position of ddCTP via an acetylene-phenyl-oxyethyleneamino linkage. This nucleotide derivative was used in DNA sequencing with Taq polymerase containing an R660S mutation. The synthesis of a number of nucleoside/nucleotide derivs. containing various rigid linkers is described.

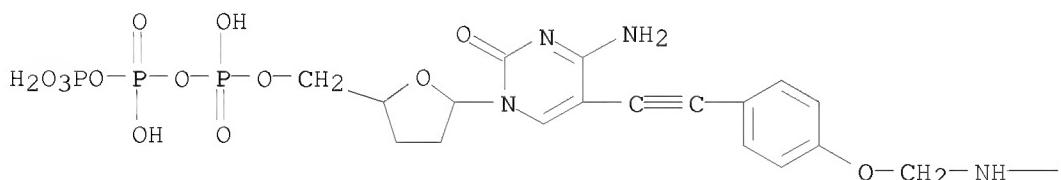
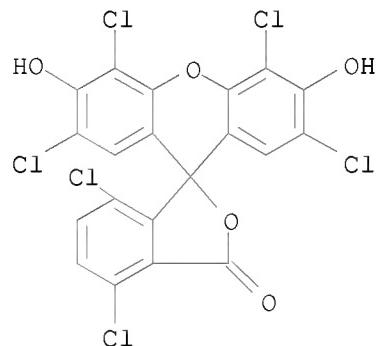
IT 241127-44-6P

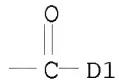
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)  
(DNA sequencing with; nucleotide compds. including rigid linker)

RN 241127-44-6 CAPLUS

CN Cytidine 5'-(tetrahydrogen triphosphate), 2',3'-dideoxy-5-[[4-[[[[2',4,4',5',7,7'-hexachloro-3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5(or 6)-yl]carbonyl]amino]methoxy]phenyl]ethynyl]-(9CI) (CA INDEX NAME)

PAGE 1-A





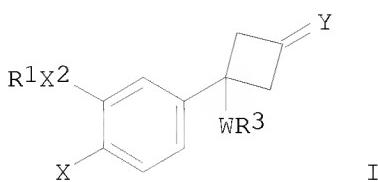
REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr 16

L4 ANSWER 16 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1999:672715 CAPLUS  
 DOCUMENT NUMBER: 131:286202  
 TITLE: Preparation of ketones, alcohols, and amines as phosphodiesterase isoenzyme denominated 4 (PDE 4) inhibiting compounds  
 INVENTOR(S): Christensen, Siegfried Benjamin, IV; Forster, Cornelia Jutta  
 PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA  
 SOURCE: PCT Int. Appl., 33 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9952847	A1	19991021	WO 1999-US7995	19990413
W: CA, JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2328250	A1	19991021	CA 1999-2328250	19990413
EP 1071645	A1	20010131	EP 1999-919814	19990413
R: BE, CH, DE, ES, FR, GB, IT, LI, NL				
JP 2002511438	T	20020416	JP 2000-543410	19990413
PRIORITY APPLN. INFO.:			US 1998-81702P	P 19980414
			WO 1999-US7995	W 19990413

OTHER SOURCE(S): MARPAT 131:286202  
 GI



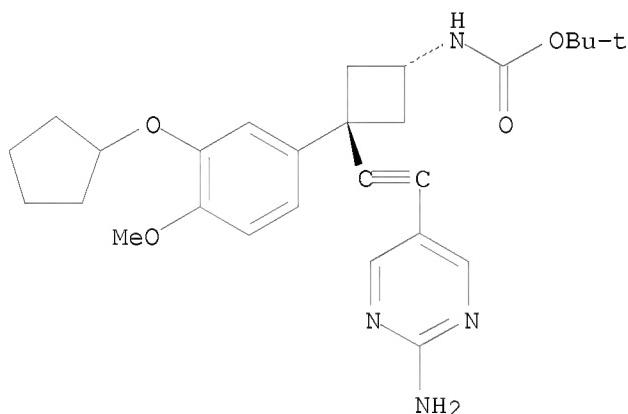
AB This invention relates to ketones, alcs. and amines I [R1 = (CR4R5)nCO2(CR4R5)mR6, (CR4R5)nCONR4(CR4R5)mR6, etc.; X = VR2, halo, NO2, NR4R5 and V = O, S(O)m'; X2 = O, NR8; R3 = CO2R14, CONR4R14, R7; Y = O, NR7, etc.; W = alkyl, alkenyl, alkynyl], represented by the likes of 3-(3-cyclopentyloxy-4-methoxyphenyl)-3-phenylethylnylcyclobutan-1-one. They are useful as PDE 4 antagonists (no data).

IT 246858-89-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of ketones, alcs., and amines as PDE 4 inhibiting compds.)

RN 246858-89-9 CAPLUS

CN Carbamic acid, [trans-3-[(2-amino-5-pyrimidinyl)ethynyl]-3-[3-(cyclopentyloxy)-4-methoxyphenyl]cyclobutyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr 15

L4 ANSWER 15 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 2000:260305 CAPLUS  
DOCUMENT NUMBER: 132:265445  
TITLE: Preparation of nucleotide compounds including a rigid linker used in DNA sequencing  
INVENTOR(S): Kahn, Shaheer H.; Rosenblum, Barnett B.; Zhen, Weiguo; Menchen, Steven M.  
PATENT ASSIGNEE(S): The Perkin-Elmer Corporation, USA  
SOURCE: PCT Int. Appl., 63 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000021974	A1	20000420	WO 1999-US12323	19990602
W: AU, CA, JP				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 6096875	A	20000801	US 1998-172789	19981014
CA 2344643	A1	20000420	CA 1999-2344643	19990602
CA 2344643	C	20070911		
AU 9946740	A	20000501	AU 1999-46740	19990602
AU 744719	B2	20020228		
EP 1121371	A1	20010808	EP 1999-930140	19990602
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2002527447	T	20020827	JP 2000-575880	19990602
JP 3900244	B2	20070404		
JP 2006306888	A	20061109	JP 2006-196282 US 1998-172789 JP 2000-575880 WO 1999-US12323	20060718 A 19981014 A3 19990602 W 19990602
PRIORITY APPLN. INFO.:				

OTHER SOURCE(S): MARPAT 132:265445

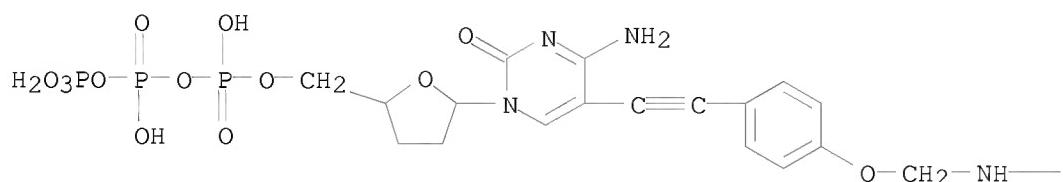
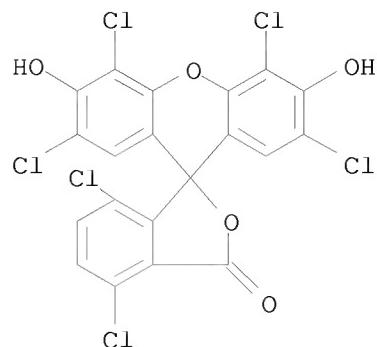
AB A nucleoside/tide compound having a rigid linker attached to the 8-position of a purine, the 7-position of a 7-deazapurine and the 5-position of a pyrimidine is disclosed. Fluorescent dyes may be attached to this linker and the fluorescent nucleotide used in primer extension reactions. Thus, the fluorescein dye HEX-1 was attached to the 5-position of ddCTP via an acetylene-phenyl-oxyethyleneamino linkage. This nucleotide derivative was used in DNA sequencing with Taq polymerase containing an R660S mutation. The synthesis of a number of nucleoside/nucleotide derivs. containing various rigid linkers is described.

IT 241127-44-6P  
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)  
(DNA sequencing with; preparation of nucleotide compds. including a rigid linker used in DNA sequencing)

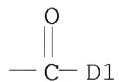
RN 241127-44-6 CAPLUS

CN Cytidine 5'-(tetrahydrogen triphosphate), 2',3'-dideoxy-5-[[4-[[[[2',4,4',5',7,7'-hexachloro-3',6'-dihydroxy-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5(or 6)-yl]carbonyl]amino]methoxy]phenyl]ethynyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr 14

L4 ANSWER 14 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:90025 CAPLUS

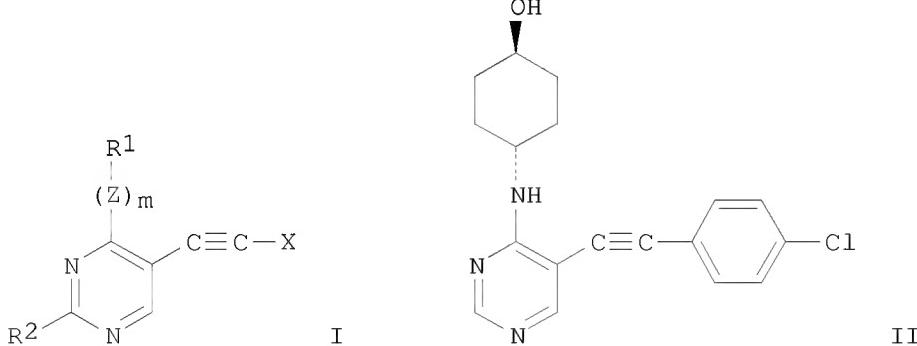
DOCUMENT NUMBER: 136:151172

TITLE: Preparation of 5-(arylalkynyl)pyrimidines having

INVENTOR(S): neurotrophic activity for the treatment of  
neurodegenerative and other neurological disorders  
Beauchamp, Lilia; Krenitsky, Thomas A.; Kelley, James  
L.  
PATENT ASSIGNEE(S): Krenitsky Pharmaceuticals, Inc., USA  
SOURCE: PCT Int. Appl., 60 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002008205	A1	20020131	WO 2001-US23088	20010720
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2416442	A1	20020131	CA 2001-2416442	20010720
AU 2001073574	A	20020205	AU 2001-73574	20010720
EP 1303495	A1	20030423	EP 2001-952859	20010720
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004504386	T	20040212	JP 2002-514111	20010720
US 20040087789	A1	20040506	US 2003-333447	20030627
US 7205297	B2	20070417		
PRIORITY APPLN. INFO.:			US 2000-220348P	P 20000724
			WO 2001-US23088	W 20010720

OTHER SOURCE(S): MARPAT 136:151172  
GI



AB Title compds. I [wherein Z = O, NH, or S; m = 0-1; R1 = (un)substituted (alkyl)a((hetero)cycloalkyl or (hetero)aryl)b(alkyl)c; a, b, and c = independently 0-1 and a + b + c ≥ 1, with provisos; R2 = H, NH<sub>2</sub>, or NHCOR<sub>3</sub>; R3 = H or alkyl; X = (un)substituted aryl; and pharmaceutically acceptable esters, amides, salts, or solvates thereof] were prepared Pharmaceutical compns. which contain I, methods for their preparation, and their use in therapy, particularly in the treatment of neurodegenerative or other neurol. disorders of the central and peripheral nervous systems,

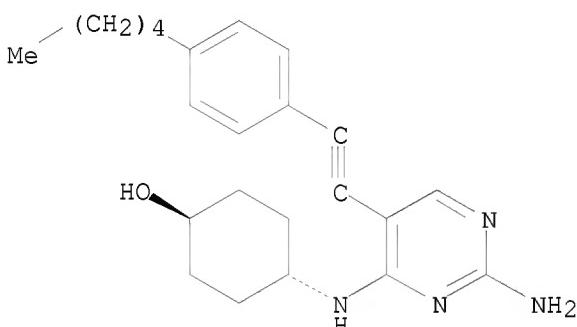
including age related cognitive disorders such as senility and Alzheimer's disease, nerve injuries, peripheral neuropathies, and seizure disorders such as epilepsy, are disclosed. For example, 4-chloro-5-(4-chlorophenylethynyl)pyrimidine (preparation given) was coupled with (trans)-4-amino cyclohexanol•HCl using TEA and MeCN in CH<sub>2</sub>C<sub>12</sub> to afford II. The latter increased the choline acetyltransferase (ChAT) activity relative to nerve growth factor (NGF) alone with EC<sub>2x</sub> of 0.2 μM.

IT 393856-10-5P, 2-Amino-4-(4-trans-hydroxycyclohexylamino)-5-(4-n-pentylphenylethynyl)pyrimidine 393856-26-3P,  
 2-Amino-5-(4-propylphenylethynyl)-4-(4-trans-hydroxycyclohexylamino)pyrimidine 393856-79-6P, 5-(4-Acetamidophenylethynyl)-2-amino-4-(4-trans-hydroxycyclohexylamino)pyrimidine 393857-35-7P,  
 5-(4-Acetamidophenylethynyl)-2-amino-4-(4-trans-hydroxycyclohexylamino)pyrimidine hydrochloride 393857-43-7P,  
 2-Amino-4-(4-trans-hydroxycyclohexylamino)-5-(4-propylphenylethynyl)pyrimidine hydrochloride  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (CNS agent; preparation of (arylalkynyl)pyrimidines having neurotrophic activity for the treatment of neurodegenerative and other neurol. disorders)

RN 393856-10-5 CAPLUS

CN Cyclohexanol, 4-[(2-amino-5-[2-(4-pentylphenyl)ethynyl]-4-pyrimidinyl]amino]-, trans- (CA INDEX NAME)

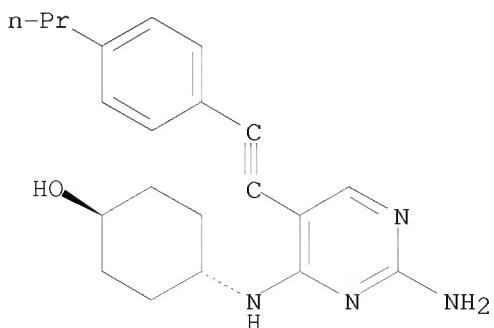
Relative stereochemistry.



RN 393856-26-3 CAPLUS

CN Cyclohexanol, 4-[(2-amino-5-[2-(4-propylphenyl)ethynyl]-4-pyrimidinyl]amino]-, trans- (CA INDEX NAME)

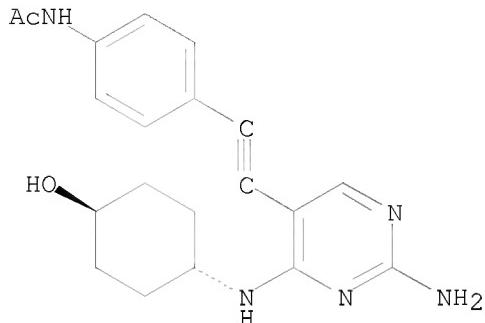
Relative stereochemistry.



RN 393856-79-6 CAPLUS

CN Acetamide, N-[4-[2-[2-amino-4-[(trans-4-hydroxycyclohexyl)amino]-5-pyrimidinyl]ethynyl]phenyl]- (CA INDEX NAME)

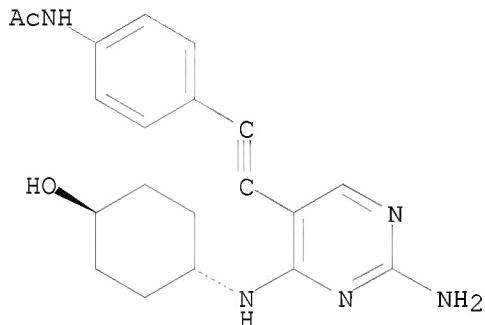
Relative stereochemistry.



RN 393857-35-7 CAPLUS

CN Acetamide, N-[4-[2-[2-amino-4-[(trans-4-hydroxycyclohexyl)amino]-5-pyrimidinyl]ethynyl]phenyl]-, hydrochloride (1:1) (CA INDEX NAME)

Relative stereochemistry.

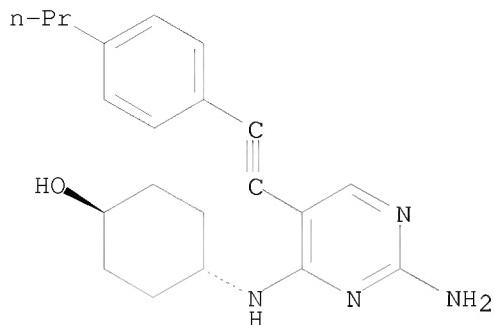


● HCl

RN 393857-43-7 CAPLUS

CN Cyclohexanol, 4-[[2-amino-5-[2-(4-propylphenyl)ethynyl]-4-pyrimidinyl]amino]-, hydrochloride (1:1), trans- (CA INDEX NAME)

Relative stereochemistry.



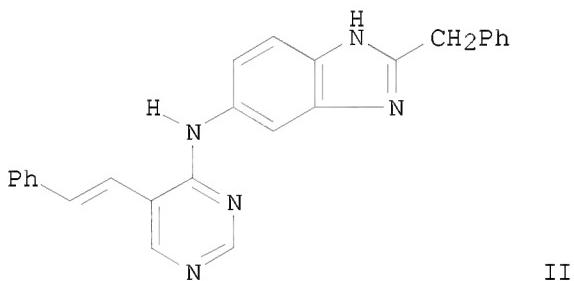
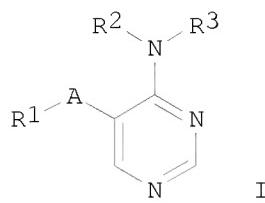
● HCl

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

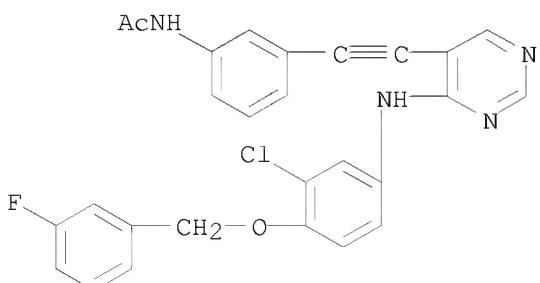
=> d ibib abs hitstr 13

L4 ANSWER 13 OF 18 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2005:158661 CAPLUS  
 DOCUMENT NUMBER: 142:240460  
 TITLE: Preparation of pyrimidine derivatives as ErbB kinase inhibitors  
 INVENTOR(S): Reno, Michael John; Stevens, Kirk Lawrence; Waterson, Alex Gregory; Zhang, Yuemei  
 PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA  
 SOURCE: PCT Int. Appl., 132 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005016914	A1	20050224	WO 2004-US26251	20040811
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1654251	A1	20060510	EP 2004-781004	20040811
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, HR				
JP 2007502298	T	20070208	JP 2006-523388	20040811
US 20060205740	A1	20060914	US 2006-568052	20060210
PRIORITY APPLN. INFO.:			US 2003-495180P	P 20030814
			WO 2004-US26251	W 20040811
OTHER SOURCE(S):	CASREACT 142:240460; MARPAT 142:240460			

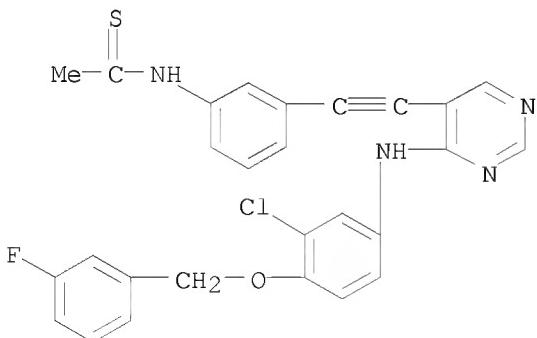


- AB Title compds. I [wherein A = alkenylene, alkynylene; R = alkylene; R1 = -(Z)-(Z1)m-(Z2)n; Z = hetero/aryl, hetero/arylene; Z1 = CH2 where m = 0-1; Z2 = OH and derivs., halo, CN, CONH2 and derivs. or heterocyclyl, where n = 0-1, etc.; R2 = H, alkyl; R3 = -(Q)-(Q1)r-(Q2); Q = hetero/arylene; Q1 = O, where r = 0-1; Q2 = arylalkyl, hetero/aryl; and their salts, solvates, and physiol. functional derivs.] were prepared as ErbB kinase inhibitors for treating cancer. Thus, reacting 2-benzyl-N-(5-vinylpyrimidin-4-yl)-1H-benzimidazol-5-amine (preparation given) with Ph iodide gave pyrimidine II in 8%. I showed inhibitory activity vs. EGFR, ErbB-2, and ErbB-4 protein tyrosine kinases with a pIC<sub>50</sub> ≥ 5.0. I are useful in the treatment of diseases associated with inappropriate ErbB family kinase activity.
- IT 845657-39-8P, N-[3-[[4-[[3-Chloro-4-[(3-fluorobenzyl)oxy]phenyl]amino]pyrimidin-5-yl]ethynyl]phenyl]acetamide  
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(drug candidate; preparation of pyrimidines as ErB kinase inhibitors)
- RN 845657-39-8 CAPLUS
- CN Acetamide, N-[3-[2-[4-[[3-chloro-4-[(3-fluorophenyl)methoxy]phenyl]amino]-5-pyrimidinyl]ethynyl]phenyl]- (CA INDEX NAME)

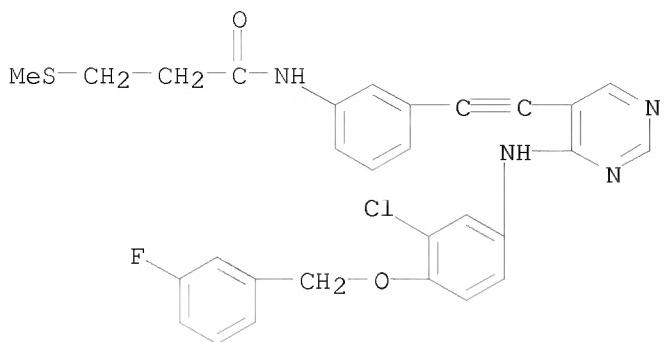


IT 845657-40-1P, N-[3-[[4-[(3-fluorobenzyl)oxy]phenyl]amino]pyrimidin-5-yl]ethynyl]phenyl]ethanethioamide  
 e 845657-49-0P, N-[3-[[4-[(3-Chloro-4-[(3-fluorobenzyl)oxy]phenyl)amino]pyrimidin-5-yl]ethynyl]phenyl]-3-(methylthio)propanamide 845657-52-5P, N-[3-[[4-[(3-Chloro-4-[(3-fluorobenzyl)oxy]phenyl)amino]pyrimidin-5-yl]ethynyl]phenyl]guanidine 845657-63-8P, N-[3-[[4-[(3-Chloro-4-[(3-fluorobenzyl)oxy]phenyl)amino]pyrimidin-5-yl]ethynyl]phenyl]-2-(2-methoxyethoxy)acetamide 845657-64-9P, N-[3-[[4-[(2-Benzyl-1H-benzimidazol-5-yl)amino]pyrimidin-5-yl]ethynyl]phenyl]acetamide 845657-65-0P, N1-[3-[[4-[(3-Chloro-4-[(3-fluorobenzyl)oxy]phenyl)amino]pyrimidin-5-yl]ethynyl]phenyl]- $\beta$ -alaninamide 845657-66-1P, N-[3-[[4-[(3-Chloro-4-[(3-fluorobenzyl)oxy]phenyl)amino]pyrimidin-5-yl]ethynyl]phenyl]-2-(methylsulfonyl)acetamide 845657-67-2P, N-[3-[[4-[(4-Benzylphenyl)amino]pyrimidin-5-yl]ethynyl]phenyl]acetamide 845657-68-3P, N-[3-[[4-[(4-Phenoxyphenyl)amino]pyrimidin-5-yl]ethynyl]phenyl]acetamide 845657-69-4P, N-[3-[[4-[(1-Benzyl-1H-indazol-5-yl)amino]pyrimidin-5-yl]ethynyl]phenyl]acetamide 845657-74-1P, N-[6-[[2-[(4-[(3-Chloro-4-[(3-fluorobenzyl)oxy]anilino)pyrimidin-5-yl]ethynyl]pyridin-2-yl]acetamide 845657-76-3P, 2-Chloro-N-[6-[[4-[(3-chloro-4-[(3-fluorobenzyl)oxy]anilino)-5-pyrimidinyl]ethynyl]-2-pyridinyl]-2,2-difluoroacetamide 845657-77-4P, N-[6-[[4-[(3-Chloro-4-[(3-fluorobenzyl)oxy]anilino)-5-pyrimidinyl]ethynyl]-2-pyridinyl]-4-(dimethylamino)butanamide 845657-78-5P, Methyl 4-[[6-[[4-[(3-chloro-4-[(3-fluorobenzyl)oxy]anilino)-5-pyrimidinyl]ethynyl]-2-pyridinyl]amino]-4-oxobutanoate 845657-80-9P, N-[3-Chloro-4-[(3-fluorobenzyl)oxy]phenyl]-5-[[6-[[2-(methylsulfonyl)ethyl]amino]-2-pyridinyl]ethynyl]-4-pyrimidinamine 845658-24-4P, 2-[[4-[(3-Chloro-4-[(3-fluorobenzyl)oxy]phenyl)amino]pyrimidin-5-yl]ethynyl]-4-[[2-(methylsulfonyl)ethyl]amino]pyrimidine-5-carbonitrile 845658-26-6P, N-[6-[[4-[(3-Chloro-4-[(3-fluorobenzyl)oxy]phenyl)amino]pyrimidin-5-yl]ethynyl]pyridin-2-yl]-2,2,2-trifluoroacetamide  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (drug candidate; preparation of pyrimidines as ErB kinase inhibitors)

RN 845657-40-1 CAPLUS  
 CN Ethanethioamide, N-[3-[[2-[(4-[(3-chloro-4-[(3-fluorophenyl)methoxy]phenyl)amino]-5-pyrimidinyl]ethynyl]phenyl]- (CA INDEX NAME)

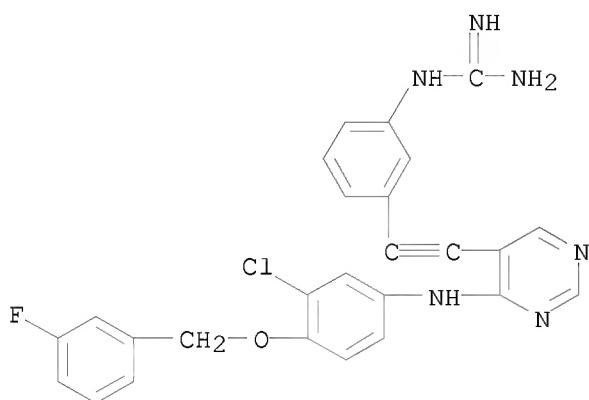


RN 845657-49-0 CAPLUS  
 CN Propanamide, N-[3-[[2-[(4-[(3-chloro-4-[(3-fluorophenyl)methoxy]phenyl)amino]-5-pyrimidinyl]ethynyl]phenyl]-3-(methylthio)- (CA INDEX NAME)



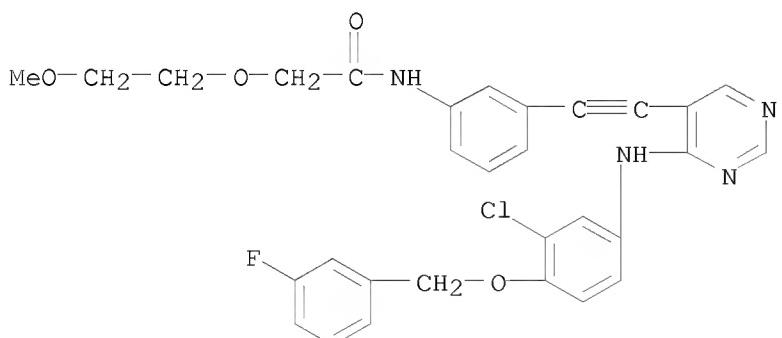
RN 845657-52-5 CAPLUS

CN Guanidine, N-[3-[2-[4-[[3-chloro-4-[(3-fluorophenyl)methoxy]phenyl]amino]-5-pyrimidinyl]ethynyl]phenyl]- (CA INDEX NAME)



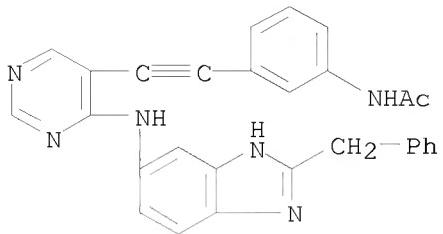
RN 845657-63-8 CAPLUS

CN Acetamide, N-[3-[2-[4-[[3-chloro-4-[(3-fluorophenyl)methoxy]phenyl]amino]-5-pyrimidinyl]ethynyl]phenyl]-2-(2-methoxyethoxy)- (CA INDEX NAME)



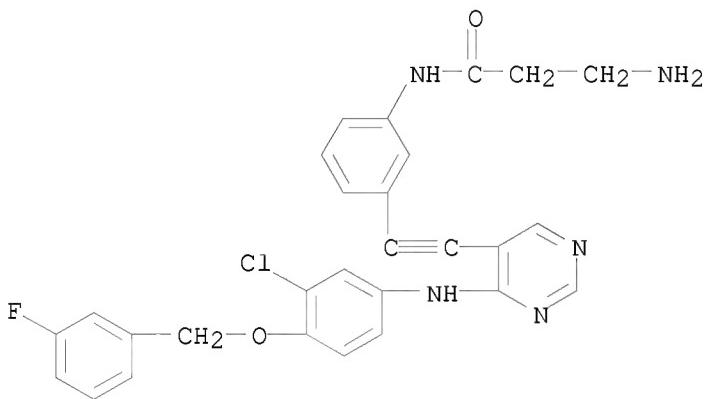
RN 845657-64-9 CAPLUS

CN Acetamide, N-[3-[2-[4-[[2-(phenylmethyl)-1H-benzimidazol-6-yl]amino]-5-pyrimidinyl]ethynyl]phenyl]- (CA INDEX NAME)



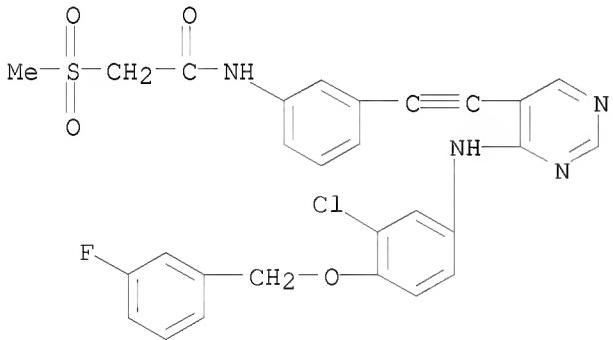
RN 845657-65-0 CAPLUS

CN Propanamide, 3-amino-N-[3-[2-[4-[(3-chloro-4-[(3-fluorophenyl)methoxy]phenyl]amino]-5-pyrimidinyl]ethynyl]phenyl]- (CA INDEX NAME)



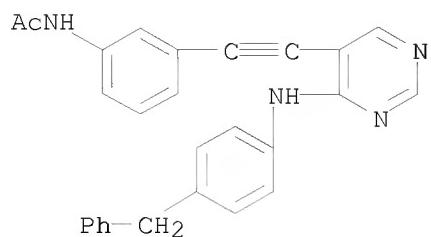
RN 845657-66-1 CAPLUS

CN Acetamide, N-[3-[2-[4-[(3-chloro-4-[(3-fluorophenyl)methoxy]phenyl]amino]-5-pyrimidinyl]ethynyl]phenyl]-2-(methylsulfonyl)- (CA INDEX NAME)

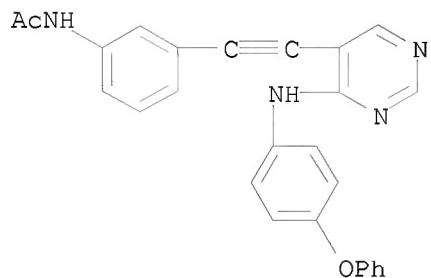


RN 845657-67-2 CAPLUS

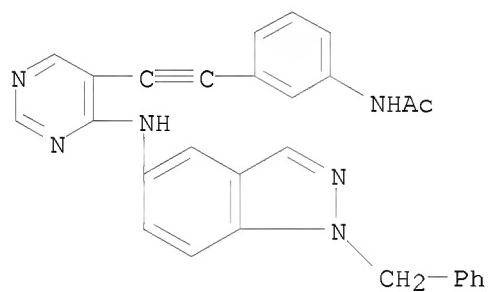
CN Acetamide, N-[3-[2-[4-[(4-(phenylmethyl)phenyl]amino]-5-pyrimidinyl]ethynyl]phenyl]- (CA INDEX NAME)



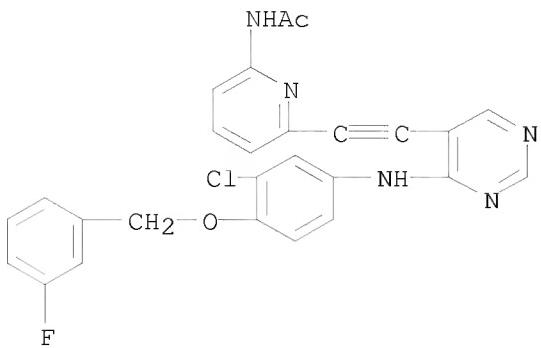
RN 845657-68-3 CAPLUS  
 CN Acetamide, N-[3-[2-[4-[(4-phenoxyphenyl)amino]-5-pyrimidinyl]ethynyl]phenyl]- (CA INDEX NAME)



RN 845657-69-4 CAPLUS  
 CN Acetamide, N-[3-[2-[4-[[1-(phenylmethyl)-1H-indazol-5-yl]amino]-5-pyrimidinyl]ethynyl]phenyl]- (CA INDEX NAME)

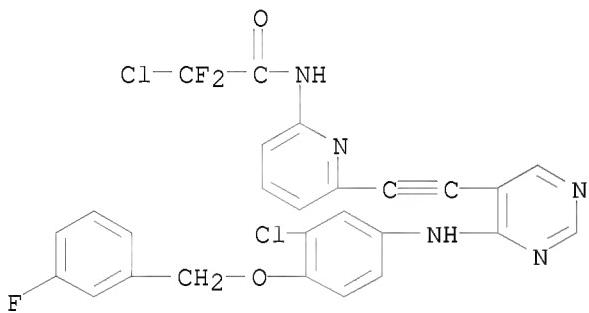


RN 845657-74-1 CAPLUS  
 CN Acetamide, N-[6-[2-[4-[[3-chloro-4-[(3-fluorophenyl)methoxy]phenyl]amino]-5-pyrimidinyl]ethynyl]-2-pyridinyl]- (CA INDEX NAME)



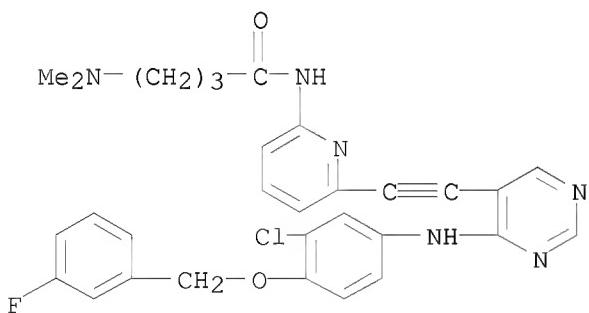
RN 845657-76-3 CAPLUS

CN Acetamide, 2-chloro-N-[6-[2-[4-[[3-chloro-4-[(3-fluorophenyl)methoxy]phenyl]amino]-5-pyrimidinyl]ethynyl]-2-pyridinyl]-2,2-difluoro- (CA INDEX NAME)



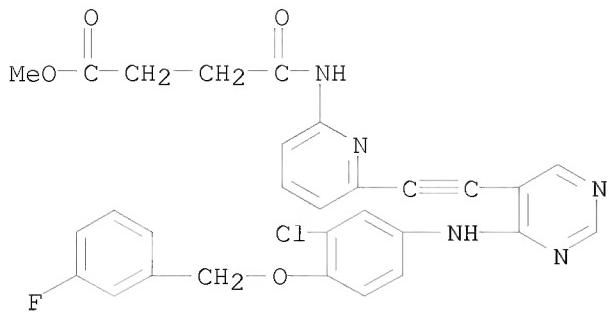
RN 845657-77-4 CAPLUS

CN Butanamide, N-[6-[2-[4-[[3-chloro-4-[(3-fluorophenyl)methoxy]phenyl]amino]-5-pyrimidinyl]ethynyl]-2-pyridinyl]-4-(dimethylamino)- (CA INDEX NAME)



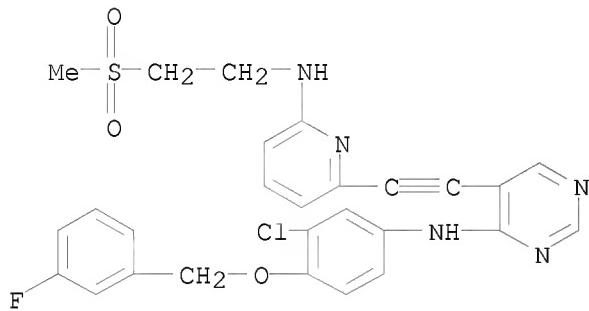
RN 845657-78-5 CAPLUS

CN Butanoic acid, 4-[[6-[2-[4-[[3-chloro-4-[(3-fluorophenyl)methoxy]phenyl]amino]-5-pyrimidinyl]ethynyl]-2-pyridinyl]amino]-4-oxo-, methyl ester (CA INDEX NAME)



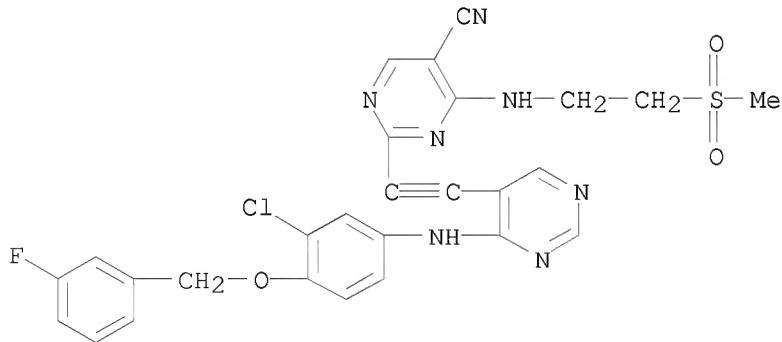
RN 845657-80-9 CAPLUS

CN 4-Pyrimidinamine, N-[3-chloro-4-[(3-fluorophenyl)methoxy]phenyl]-5-[2-[(2-(methylsulfonyl)ethyl)amino]-2-pyridinyl]ethynyl- (CA INDEX NAME)



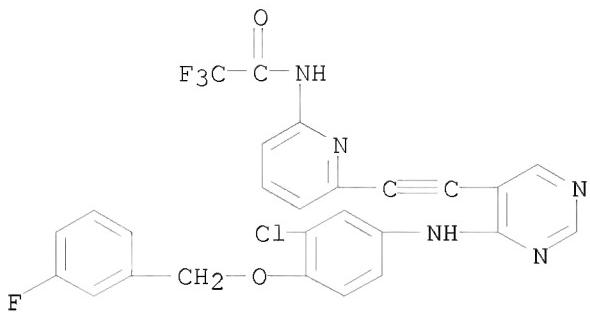
RN 845658-24-4 CAPLUS

CN 5-Pyrimidinecarbonitrile, 2-[2-[4-[(3-chloro-4-[(3-fluorophenyl)methoxy]phenyl)amino]-5-pyrimidinyl]ethynyl]-4-[(2-(methylsulfonyl)ethyl)amino]- (CA INDEX NAME)



RN 845658-26-6 CAPLUS

CN Acetamide, N-[6-[2-[4-[(3-chloro-4-[(3-fluorophenyl)methoxy]phenyl)amino]-5-pyrimidinyl]ethynyl]-2-pyridinyl]-2,2,2-trifluoro- (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> logoff

ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF

LOGOFF? (Y)/N/HOLD:Y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	37.50	216.99
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-4.80	-4.80

STN INTERNATIONAL LOGOFF AT 10:41:24 ON 08 SEP 2008